Modeling Solidification, Elasticity and Structural Stability using Phase Field Crystals

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Abstract

Elastic and plastic deformations often play a significant role in determining the microstructures that emerge during non-equilibrium processing. The microstructures produced in these phenomena are important since they can significantly alter material properties. In a prior work a phase field crystal (PFC) model [1] was developed to examine such phenomena in pure materials. In this talk an extension of the PFC model to binary alloys is presented and several applications are discussed.

Binary Phase Field Crystals

Elastic and plastic deformations are intimately related to the creation and properties of material microstructures. For example in polycrystalline materials, dislocation creation, interactions, energy and motion all play a crucial role in determining grain size distributions and yield strength. In a previous work [1] a phase field crystal model was developed to examine the influence of elastic and plastic deformations on non-equilibrium processes and material properties. This model describes the local mass density on diffusive time but atomic length scales and consequently lies in between microscopic and standard mesoscopic continuum descriptions. The advantage of describing phenomena on microscopic length scales is that many important features that are difficult to include in continuum theories, such as elastic deformation, dislocation nucleation and motion, multiple orientations and free surfaces are automatically included. While molecular descriptions also include these features, such approaches are limited by microscopic time scales (~ ps) and thus cannot study many important phenomena on realistic time scales. The PFC model was developed by exploiting the large separation of time scales between microscopic (i.e., phonon modes) and diffusive ones and by recognizing that free energies minimized by spacially periodic fields automatically contain elastic and plastic energy.

While the pure PFC model describes many interesting phenomena, most industrially significant materials contain multiple components which influence material properties and microstructure formation. To complicate matters many crystal properties, such as elastic constants and lattice spacing, are dependent on concentration. To model elastic and plastic deformation in binary alloys the pure PFC model [1] was combined with a model of eutectic solidification [2]. This new model describes the dynamics of the time averaged density field for two species ('A' and 'B') and was constructed such that the concentration dependence of the elastic constants and atomic spacing can be easily tuned. A phase diagram derived from this model is shown in Fig. (1). The asymmetry in the diagram arises from using a non-zero solute expansion.

Figure 1: In this figure the hatched areas correspond to coexistence regions.

To show that the model contains the correct interface dynamics the binary PFC model was used to study single crystal growth from a supercooled liquid in both solid/solid and liquid/liquid coexistence regions. Figure (2a) depicts growth in the former case where a lamellar pattern emerges in the growing crystal. In the later case a dendritic structure naturally emerges as shown in Fig. (2b). While not a definitive test, in both cases the expected structures appeared. Perhaps more interestingly these simulations show how the binary PFC model can resolve such structures down to microscopic length scales (see insets in Fig. (2)).

While many models have been developed that can produce the overall patterns shown in Fig. (2) the binary PFC model also simultaneously incorporates all the elastic features of the pure PFC model. To illustrate this point,
the heterogeneous nucleation and growth of multiple crystals in a supercooled liquid was considered. The results are shown in Figs. (3), (4) and (5) for the mass density, composition and energy density respectively. Figure (3) highlights multiple crystal orientations, liquid/crystal surfaces, dislocations and although more difficult to discern different lattice parameters in the two different crystal phases (both triangular lattices). Figure (4) shows discontinuities in the composition (or ‘domain walls’) between two different crystal phases and the crystal/liquid surfaces. Finally Fig. (5) shows three different energy states for the liquid and two different crystal phases, domain wall energy associated with compositional discontinuities, dislocation cores and grain boundaries. Comparison of all figures also shows dislocations collecting at crystal/crystal domain walls. This occurs due to the strain arises from the lattice constant mismatch (i.e., from a non-zero solute expansion coefficient).

In summary a binary PFC model has been developed that incorporates all the physics of binary alloy solidification dynamics and elastic and plastic deformation. Additional applications, including the influence of composition on epitaxial growth, will be discussed.

References
